



ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 20 21 22 23 24 25 26 27
28 29 30 31

ring bonds :

1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 7-11 8-9 8-14 9-10 11-12 12-13 13-14 13-15
14-18 15-16 16-17 17-18 20-21 20-25 21-22 22-23 23-24 24-25 26-27 26-31 27-28
28-29 29-30 30-31

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 7-11 8-9 8-14 9-10 11-12 12-13 13-14 13-15
14-18 15-16 16-17 17-18 26-27 26-31 27-28 28-29 29-30 30-31

normalized bonds :

20-21 20-25 21-22 22-23 23-24 24-25

G1:O,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 34:Atom